

PORTLAND HARBOR RI/FS

APPENDIX B

**FOOD WEB MODEL DEVELOPMENT FOR PORTLAND
HARBOR AQUATIC SYSTEMS
FEASIBILITY STUDY**

DRAFT

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LIST OF ACRONYMS

COC	Contaminant of Concern
DDE	4,4'-dichloro-diphenyl-dichloroethene
EPA	U.S. Environmental Protection Agency
FWM	Food Web Model
Kow	Octanol-Water Partition Coefficient
LWG	Lower Willamette Group
ng/L	nanograms per liter
PCBs	Polychlorinated Biphenyls
PRGs	Preliminary Remediation Goals
RI/FS	Remedial Investigation/Feasibility Study
RM	River Mile
TOC	Total Organic Carbon
TSS	Total Suspended Solids
µg/kg dw	microgram per kilogram dry weight

EXECUTIVE SUMMARY

This appendix provides a description of the process utilized to develop a food web model (FWM) for the Portland Harbor Superfund Site.

1.0 FOOD WEB MODEL DEVELOPMENT BACKGROUND

The Lower Willamette Group (LWG) developed a modeling approach to assist with developing sediment Preliminary Remediation Goals (PRGs) based on protection of upper trophic-level ecological receptors, illustrating uncertainties in these PRGs, and estimating risk reduction for various remedial alternatives. The model was also used to help establish appropriate sediment PRGs for protection of people that may take and consume fish and shellfish from the lower Willamette River, and to assess risk reduction. The FWM has not previously been summarized in a single location to date, and understanding of development and use of this model currently requires examination of several documents written from 2005 to 2012. This appendix provides a succinct description of model development. Note that the information summarized is from several draft reports and their appendices and attachments. None of these reports have been approved by EPA to date.

The FWM was developed iteratively over several years, but the process can be broken down into three phases for discussion purposes.

- Initially, a FWM was selected that appeared to provide the best fit to available tissue data. This process included a qualitative analysis of models that could be useful, followed by a quantitative comparison between the Arnot and Gobas model (2004) and the Trophic Trace model (USACE 2003). Polychlorinated biphenyls (PCBs) and 4,4'-dichloro-diphenyl-dichloroethene (DDE) tissue data from Round 1 and 2 field investigations were used in this comparison. The sensitivity of the model to selected input parameters was part of this comparison, as was initial evaluation of model uncertainty. The Arnot and Gobas model was judged to be the better predictor of tissue concentrations (Windward Environmental 2005).
- The model developed by Arnot and Gobas (2004) was the focus of more detailed evaluation to develop a calibrated steady state model. Calibration against tissue data from Round 1 and 2 field investigations was accomplished by identifying parameter distributions that reflect the range of possible values for many model inputs. Literature values were used to assign these distributions in many cases, but site-specific information was used whenever it was available. Calibrated input parameters that provide an overall reasonable best fit to empirical tissue data were identified from results of multiple model runs. For these runs, point estimates from input distributions were randomly chosen (Windward Environmental 2009).
- Final model development converted the steady-state FWM to a dynamic model by integrating it with a fate and transport model (QEAFAFATE) developed independently. The combination of the FWM and QEAFAFATE allowed tissue concentrations to be predicted over different temporal and spatial scales. The combined FWM and QEAFAFATE models are referred to as the *dynamic bioaccumulation model*. In its final iteration, this model was used to assess risk

reduction under no action and various remedial alternatives (Windward Environmental 2012).

Each of these three phases of model development is summarized in the following sections. Details of development of the final dynamic bioaccumulation model are found scattered in several documents produced between 2005 and 2012, which are cited as appropriate in the text.

1.1 SELECTION OF FOOD WEB MODEL

Following an initial evaluation of steady-state aquatic FWMs (Windward Environmental 2004), two models were selected for additional evaluation. One model was adapted from the publication by Arnot and Gobas (2004). The second, Trophic Trace (USACE 2003), is a model developed by the U.S. Army Corps of Engineers (USACE) to assist with management of dredge materials. Some input parameters for these models (e.g., sediment concentrations, sediment total organic carbon [TOC]) were derived from site-specific data, but most input parameters were literature-based. Input for species- and chemical-specific parameters are typically not available in site data sets and must be taken from published information. Input parameters are summarized in **Table B-1** and **Table B-2**. These parameters were used as input to the equations used in the Arnot and Gobas (**Table B-3**) and Trophic Trace¹ models to simulate movement of PCB and DDE through the food web.

Both models simulated bioaccumulation across several trophic groups, some represented by specific species, including:

- Phytoplankton
- Zooplankton
- Benthic infaunal filter feeders (clams, *Corbicula fluminea*)
- Benthic infaunal consumers (oligochaetes, insect larvae and amphipods)
- Epibenthic invertebrate consumers (crayfish, no species identified)
- Foraging fish (sculpin, *Cottus* sp) (Group also used to represent black crappie [*Pomoxis nigromaculatus*] and peamouth [*Mylocheilus caurinus*])
- Benthivorous fish (largescale sucker, *Catostomus macrocheilus*) (Group also used to represent brown bullhead [*Ameiurus nebulosus*])
- Omnivorous fish (common carp, *Cyprinus carpio*)
- Small piscivorous fish (smallmouth bass, *Micropterus dolomieu*)
- Large piscivorous fish (Northern Pike, *Esox lucius*)

¹ Input parameters and equations are not provided for the Trophic Trace model in this summary since it was not used for PRG development and alternatives analysis. This information is found in Windward Environmental (2005), Portland Harbor RI/FS Food Web Modeling Report (Draft), November 2005.

Performance of FWM models was compared on both site-wide and local (Swan Island Lagoon) spatial scales. Performance was judged by comparing mean measured tissue concentrations with predicted mean concentrations for all groups/species included in the food web. Mean empirical tissue concentrations were calculated from all fish tissue data available for the Harbor-wide site or lagoon areas.

Starting points for modeling were mean shallow (30 cm) sediment concentrations of PCB and DDE for either large (River Mile 1.9 to 11.8) or local (Swan Island lagoon) areas. All trophic groups/species included in the FWM models were also included in the performance evaluation as data permitted. Thus, up to ten comparisons for each model for each spatial scale were generated.

Overall, the Arnot and Gobas model outperformed Trophic Trace across several metrics. When individual trophic groups were compared, ratios of predicted to observed tissue concentrations were less in most cases for Arnot and Gobas versus Trophic Trace. Further, average ratios across all trophic groups were typically lower for the Arnot and Gobas model, and a greater number of ratios for individual trophic groups were less than targets of 5 and 2.

The basis for these latter ratios was not provided in available reports; they appear to reflect discussions between LWG and EPA for judging model performance. These target ratios indicate that the model predicted tissue concentrations within a factor of five and two, respectively. Note that, for ease of interpretation, ratios were always calculated with the larger of measured and predicted tissue concentrations in the numerator. Thus, both under- and over-predictions were expressed as positive ratios of 1 or more. Using uncalibrated input parameters, the Arnot and Gobas model tended to predict tissue concentrations that were lower than those observed in tissue data collected in Rounds 1 and 2.

It is unclear if this under-prediction reflects the structure of the FWM, the representativeness (or lack thereof) of available data or some combination. Discussion of initial FWM results did not address this issue in a substantive way. Instead, available data were assumed to accurately reflect actual tissue concentrations for species at all trophic levels, and the FWM was subsequently calibrated to these data. This approach is uncertain, but currently available data may not be sufficient to address this uncertainty quantitatively.

Based on the above comparisons, the Arnot and Gobas model was adopted for calibration (Windward Environmental 2005). Complete model code in visual basic is provided in **Attachment 1**. Modeling was completed using macro-enabled Excel workbooks.

1.2 FOOD WEB MODEL CALIBRATION

Additional development of the Arnot and Gobas FWM first focused on calibration of the model to empirical data collected during Round 1 and Round 2 field investigations (Windward Environmental 2009). Calibration involved replacing single values for many

input parameters with distributions that reflect a reasonable range of values. The model was then run many times with each run selecting input parameters randomly from input distributions². Results of these runs were used to identify combinations of input parameters that appeared to minimize differences between empirical and predicted PCB concentrations across all trophic levels. This approach did not yield a unique solution – that is, several different combinations of input parameters would yield good fits to empirical data. This issue is further addressed below.

Input distributions for the calibration exercise were developed using the following criteria:

- If site-specific data were available, estimates of mean and standard error were used to a normal distribution. Water temperature is an example of an input parameter distribution defined using site data.
- If site data were lacking, but mean and standard deviation estimates were available in the literature, these estimates were used to define a normal distribution.
- For chemicals and chemical groups, uniform distributions were used to define log octanol-water partition coefficient (K_{ow}) using data from the literature. For PCBs, site-specific data for congener composition of total PCBs was also considered to account for differing contributions for specific congeners.
- Triangular and uniform distributions were used for parameters for which mean and standard error/deviation estimates were not available. In most cases, defining these distributions involved consideration of values used in other published models and on professional judgment.
- For a number of parameters, point estimates were retained.

Detailed explanations of the derivation of input distributions for the FWM are included in Appendix D of Windward Environmental (2009).

Although distributions for many input parameters were assigned³, a sensitivity analysis that accompanied multiple model runs identified only a few parameters important in determining model fit to empirical data:

- Concentration of contaminant of concern (COC) in sediment solids (micrograms per kilogram dry weight [$\mu\text{g/kg dw}$])
- Concentration of COC in surface water (nanograms per liter [ng/L], filtered)
- Log K_{ow}

² This approach is often referred to as a stochastic or “Monte Carlo” analysis.

³ Not all input parameters were assigned distributions for the calibration exercise. In these instances, fixed input parameters were used during model calibration.

- Water temperature (degrees Celsius [°C])
- Benthic invertebrate consumer's lipid content (%)

These parameters are either defined by site-specific data, or are well studied in the literature. Thus, confidence that calibrated parameters reasonably reflect relative contributions of model parameters on FWM predictions is relatively high. That is, manipulating inputs within reasonable ranges would, for most parameters, have little impact on model performance. Uncertainty due to choice of calibrated input parameters appears to be acceptable, given the assumption that fish tissue data are representative.

An example of output from the calibrated FWM is provided as **Figure B-1**, which shows predicted (modeled) versus empirical data from the Remedial Investigation (RI) database.

After calibration, calibrated parameters (**Tables B-1, B-2, and B-4**) were used as inputs for the development of the dynamic bioaccumulation model (Windward Environmental 2009, Tables 5-10 to 5-13).

Supporting documentation is included as appendices to the Windward Environmental 2009 report.

- Appendix D: Mechanistic Model Parameterization (explains selection of parameter distributions for FWM inputs)
- Appendix E: Model Documentation (explanation of model calculations, including full model code in visual basic)
- Appendix F: Round 3 Data Compared to the Round 2 Report Mechanistic Model (updates comparisons of empirical and predicted tissue concentrations for tissue data collected in Round 3)
- Appendix G: Empirical Tissue Data for the Mechanistic Model (provides summary statistics for tissue data used in the calibration exercise)

1.3 DYNAMIC BIOACCUMULATION MODEL

The calibrated FWM generates tissue concentration estimates for steady-state conditions defined by inputs to the model. This model is useful for development of PRGs, but is not able to estimate sediment concentrations temporally and spatially. One objective of the FWM was to predict impacts of remedy on sediment COC concentrations, and to examine risk reduction across different remediation alternatives. Thus, the final stage in the development of the FWM was to connect it to a separately developed fate and transport model (QEAFATE; Windward Environmental 2012⁴).

The dynamic modeling effort focused on total PCB and, initially, PCB homologue groups (tri- to hepta-chlorinated). PCBs were used in model development since this chemical

⁴ Development of the QEAFATE model is described elsewhere in the RI.

group is ubiquitous in Portland Harbor, and contributes significantly to estimated risks throughout the aquatic system. Homologue groups were used to determine if the model could reasonably predict chemical concentrations for COCs with differing chemical characteristics, particularly different K_{ow} estimates.⁵

Output from the QEAFATE model was linked to the FWM such that the FWM would estimate tissue concentrations in monthly time steps on three different spatial scales, including:

- Entire site (River Mile [RM] 1.9 to 11.8)
- Four river segments of 2 to 3 river miles
- Individual river miles divided into east bank, west bank, and channel. The Swan Island Lagoon was modeled separately as a single unit

For example, at time zero, QEAFATE would feed input estimates for parameters such as COC concentrations in water and sediment, and water temperature to the FWM. The FWM would then calculate tissue concentrations from these values for each of the above spatial scales. QEAFATE would then send updated input estimates at time equals one month and calculations would be repeated. This process would be repeated for as many months as the analyst wished to evaluate, yielding predictions of impacts from no action or different remedial alternatives over time for the entire site, for longer river segments, for river miles by east bank, west bank and channel, and for Swan Island Lagoon.

As indicated above, inputs to the dynamic bioaccumulation model included calibrated inputs to the FWM and predicted values from the QEAFATE model. Some key inputs used in both models had to be coordinated to maintain consistency.

- Total PCBs were not modeled directly with QEAFATE and the calibrated K_{ow} was used in QEAFATE.
- Water temperatures were included in QEAFATE as an annual series of temperatures based on estimates of monthly averages. These temperatures served as input to the FWM.
- Inputs from the QEAFATE model were also used to describe dissolved COC concentrations in the water column; dissolved COC concentrations in the top 12 inches of sediment; particulate-phase contaminant COC concentrations in the top 13 inches of sediment; total suspended solids (TSS); and sediment organic carbon fraction. (TSS was predicted by an independent sediment transport model.)

Results from the development stage of the dynamic bioaccumulation model are reported in Attachment 1 of Appendix Hb of the 2012 draft Portland Harbor RI/FS (Windward

⁵ PCB homologue groups were not separately evaluated in risks assessments and were not selected as COCs for consideration in the feasibility study. Results from modeling these groups separately in the dynamic bioaccumulation model were used only to evaluate model performance across a range of K_{ow} values. They were not subsequently used in development of PRGs or for evaluation of remedial alternatives.

Environmental 2012). An example of the model output is provided in **Figure B-2**. These figures make predictions based on calibrated relationships among biotic and abiotic components of the dynamic bioaccumulation model. These predictions are predicted on the assumption that available data are adequately representative of conditions at the time that remedy implementation commences. Additional data collection and model calibration will be necessary to maintain acceptable model performance over time.

2.0 REFERENCES

Arnot JA, Gobas FAPC. 2004. A food web bioaccumulation model for organic chemicals in aquatic ecosystems, *Environ Toxicol Chem* 23:2342-2355.

USACE. 2003. Trophic Trace: A Tool for Assessing Risk from Trophic Transfer of Sediment-Associated Contaminants (online), US Army Corp of Engineers and Menzie-Cura & Associates, (Cited 3/23/2004). Available from: <http://www.wes.army.mil/el/trophictrace/index.html>

Windward Environmental. 2005. Food Web Modeling Report: Evaluating Trophic Trace and Arnot and Gobas Models for Application to the Portland Harbor Superfund Site (Draft), Portland Harbor RI/FS. November 4, 2005.

Windward Environmental. 2009. Bioaccumulation Modeling Report (Draft) and Appendices, Portland Harbor RI/FS. July 21, 2009.

Windward Environmental. 2012. Appendix Hb: Documentation for the Dynamic Bioaccumulation Model, Draft Feasibility Study, Portland Harbor RI/FS. March 2012.

Tables

Figures

Attachment 1